LIÈGE université
Sciences Appliquées

A 3-scale computational homogenisation strategy for sheet moulded compounds using material network surrogates

5th International Conference on Computational Methods for Multi-scale, Multi-uncertainty and Multi-physics Problems
CM3P 2025
July 1-4, 2025, Porto, Portugal

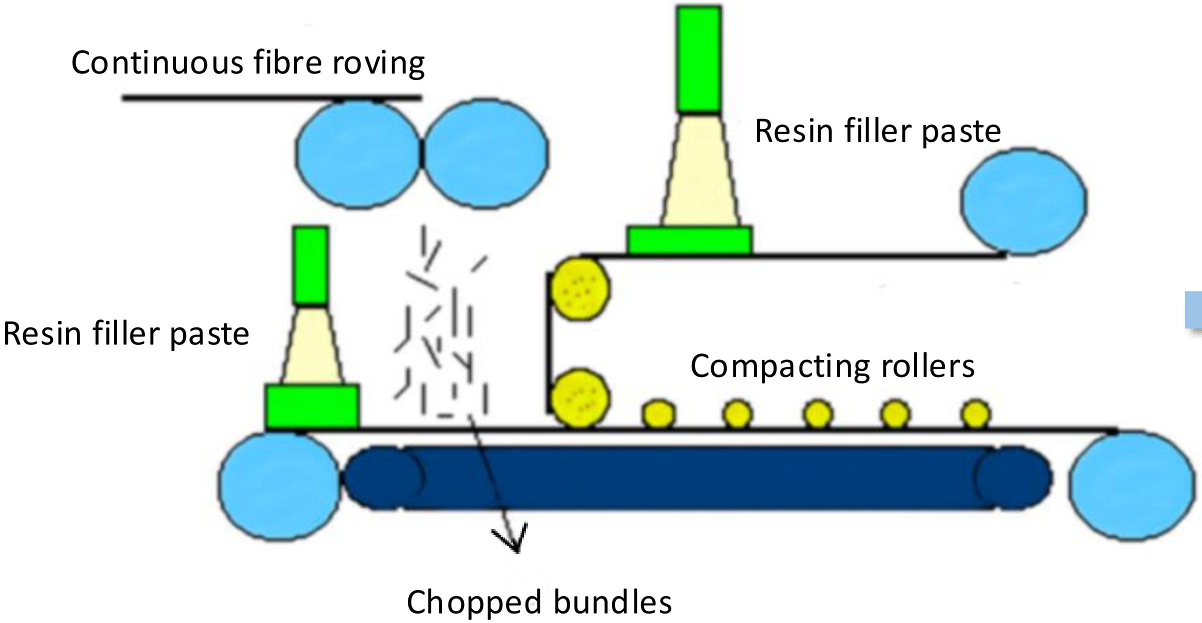
U.-K. Jinaga*, L. Wu, L. Noels
Computational & Multiscale Mechanics of Materials (CM3),
B52, Allée de la découverte 9, B4000 Liège, Belgium
http://www.ltas-cm3.ulg.ac.be/

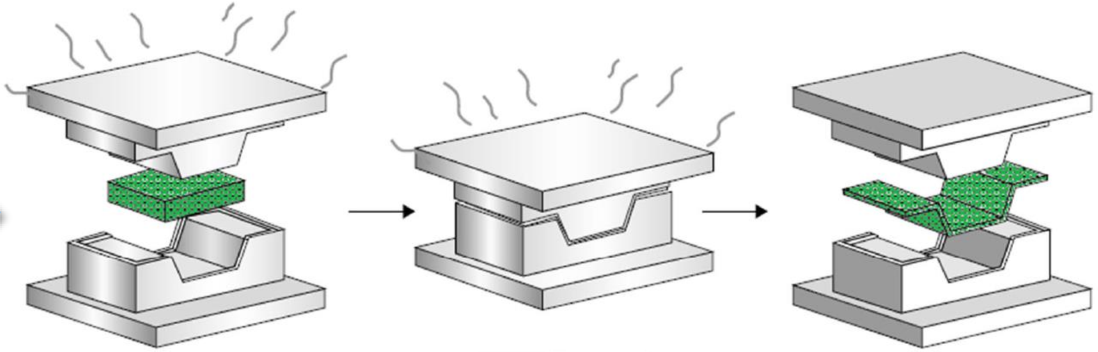
A. Kapshammer
Institute of Polymer Product Engineering (IPPE),
Johannes Kepler Universität, Linz, Austria
https://www.jku.at/institute-of-polymer-product-engineering/

K. Zulueta
Leartiker Polymer,
Xemein Hiribidea, 12 A, 48270 Markina-Xemein, Biscay, Spain
https://www.leartiker.com/polymers

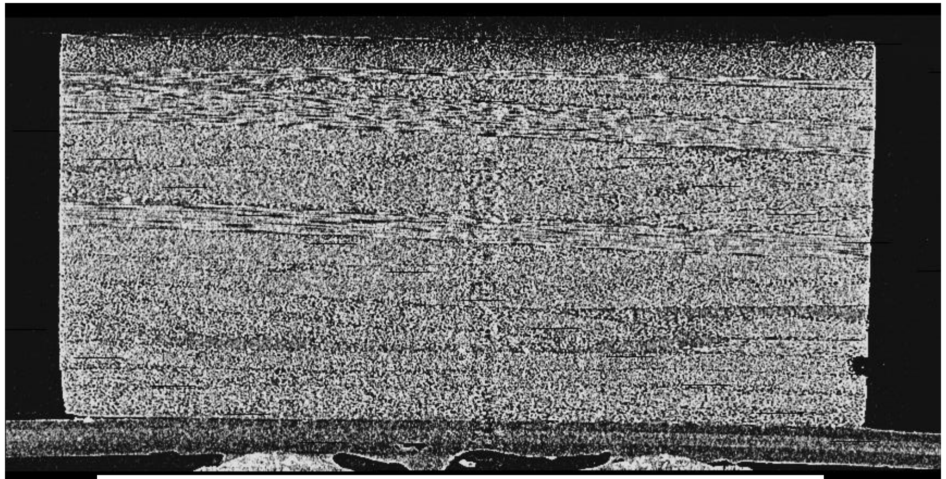
This research has been funded by the Walloon Region under the agreement no. 2010092-CARBOBRAKE in the context of the M-ERA.Net Join Call 2020. Funded by the European Union under the Grant Agreement no. 101102316. Views and opinions expressed are those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the granting authority can be held responsible for them.

Sheet Moulding Compound (SMC)





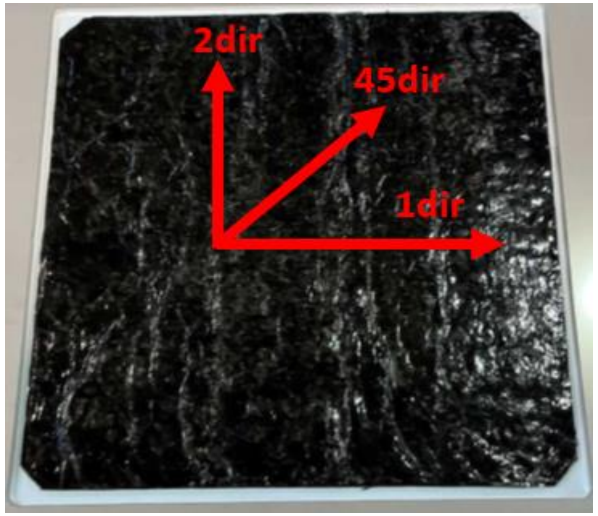
Compression Moulding
[MDC Mould 2020, Ebrahimian 2024]



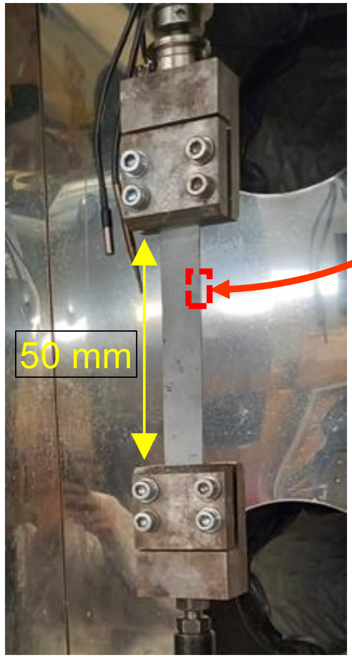
CT-scan of low flow specimen [Zulueta 2024]

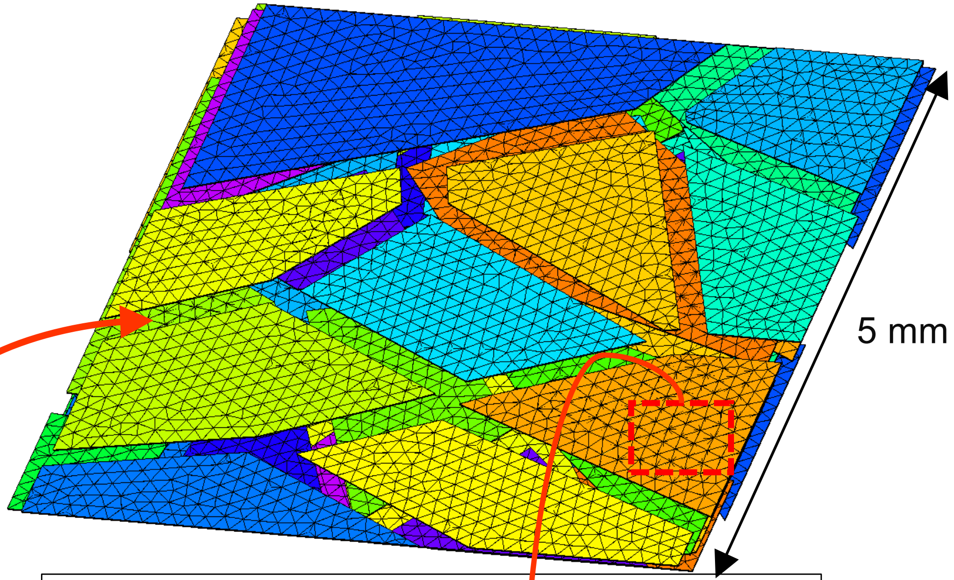
- Mitsubishi STR120N131 SMC - Vinyl ester carbon fibre 58-42% by vol. [Fidler 2024]
- Process dependant microstructure
- Low flow – random (only) in-plane orientation of fibre bundles

3 scale thermomechanical FE^3 strategy for SMC

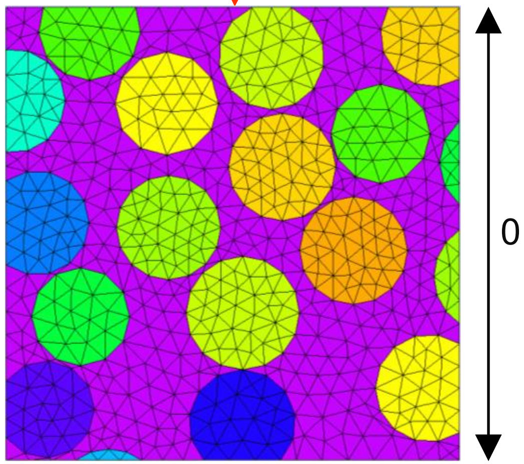


ISO 527 Sample – Flow aligned





Mesoscale RVE – Oriented Bundles in matrix

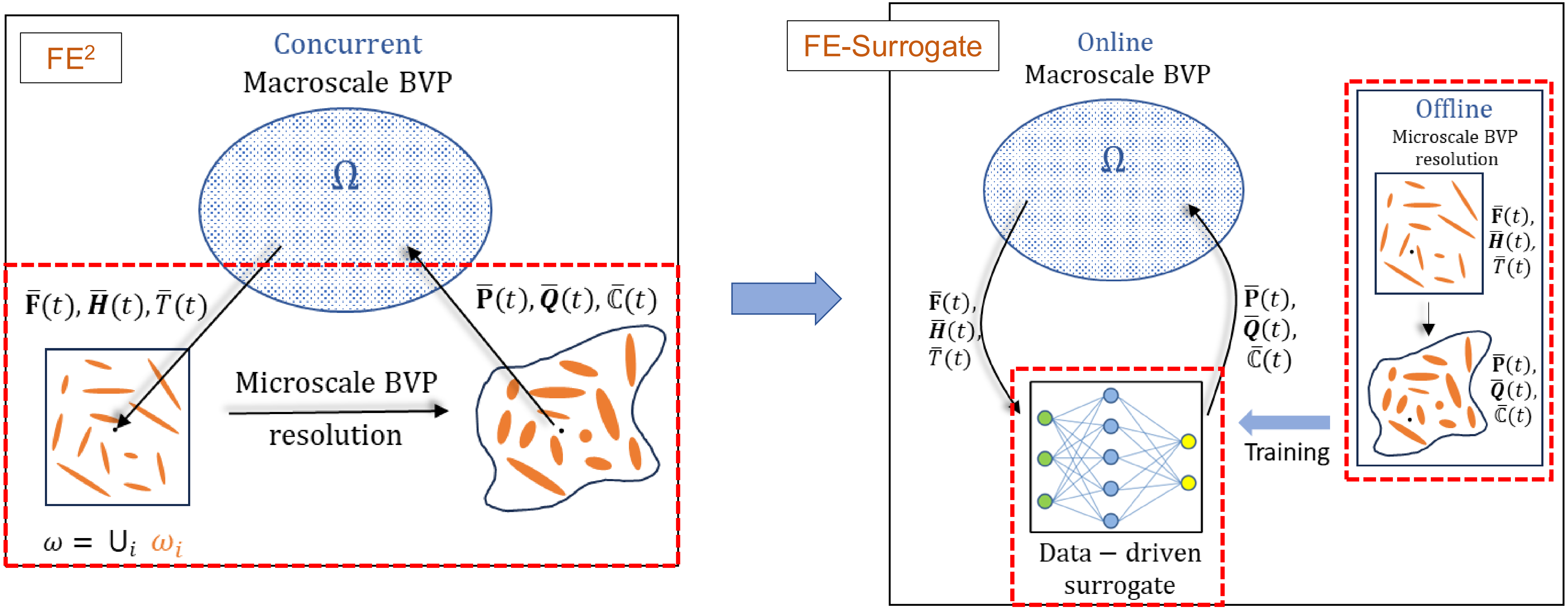


Microscale RVE – Unidirectional fibres in matrix
- 62.1% VF fibre (12 μm diameter)

Objectives

- Fast thermomechanical homogenisation using data-driven surrogates
- Extension of mesoscale surrogacy for local orientations

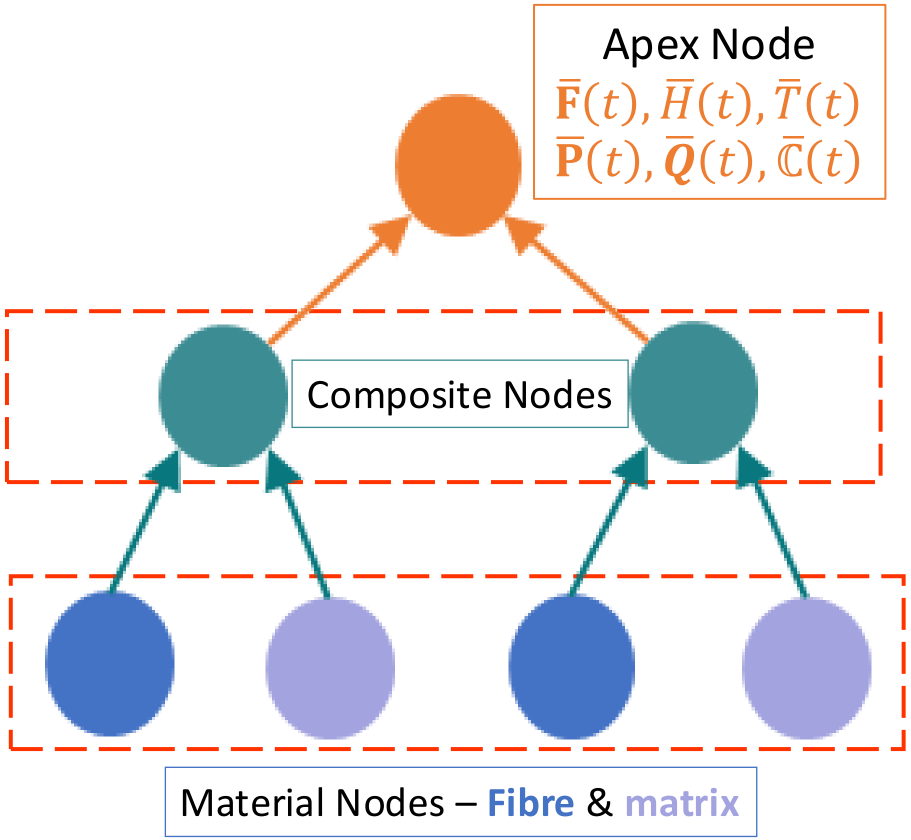
Data-driven analysis for a 2-scale thermomechanical problem



- FE computationally expensive for complex RVEs
- Replace lower scale BVP with data-driven surrogate. E.g. Deep Neural Networks (DNN), Reduced Order Models (ROM)
- DNNs cannot extrapolate, ROMs only for specific cases

Higher scale variables
$\bar{\mathbf{F}}$ - deformation gradient
$\bar{\boldsymbol{H}}$ - temperature gradient
$\bar{T}$ - temperature
$\bar{\mathbf{P}}$ - 1st PK stress
$\bar{\boldsymbol{Q}}$ - heat flux
$\bar{\mathbb{C}}$ - Constitutive matrix

Deep Material Network (DMN) [Liu 2019]



$$\begin{cases} \mathbf{P}^i\left(\mathbf{F}^i(t), T^i(t), z(\tau \le t)\right) \\ \boldsymbol{Q}^i\left(\mathbf{F}^i(t), \boldsymbol{H}^i(t), T^i(t), z(\tau \le t)\right) \end{cases}$$

$(\cdot)^i$ - Lower scale variables
z - Internal variables

How does it work?

- Simplest form – A perfect binary tree
- Phase constitutive laws at the material nodes - $\mathbb{C}_i^{l=0}$
- At the k^th composite node – Recursive calls to lower nodes

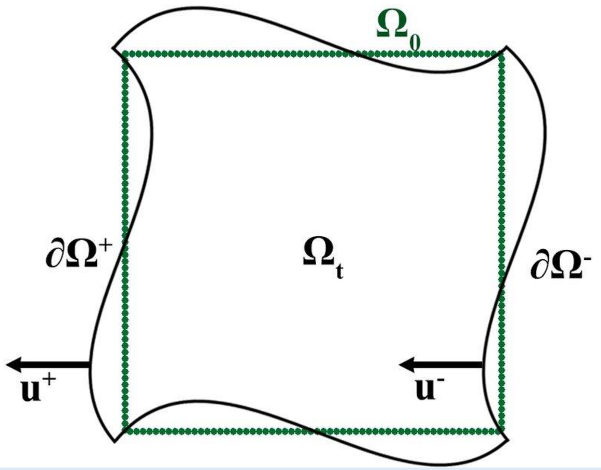
$$\mathbb{C}_k^{l=j} = \mathrm{DMN}\left(\mathbb{C}_i^{l=j-1}, \Lambda^3\right)$$

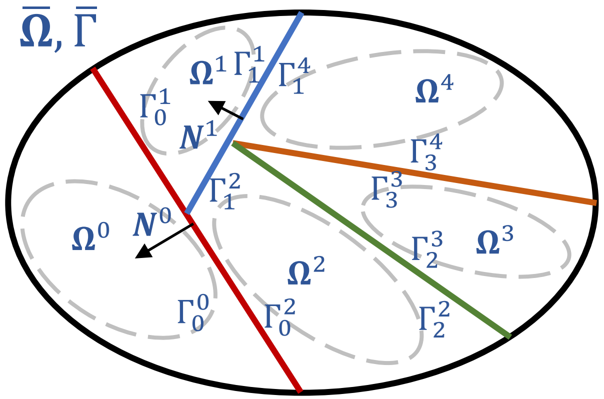
where Λ^3 is the set of trainable parameters

- Homogenised response at the apex node

Thermodynamically consistent and extrapolative!
[Liu 2019, Nguyen 2022]

Lower scale BVP → Material Network





Main Elements of the 2-scale thermomechanical problem

- 1st order expansion of $\mathcal{F}$ in $x_\mu \in \bar{\Omega}$, for $\mathcal{F} = [\mathbf{F}, \boldsymbol{H}^T]^T$

$$\mathcal{F}_\mu(x_\mu) = \bar{\mathcal{F}} + \nabla \odot \boldsymbol{\alpha}'(x_\mu)$$

where $\boldsymbol{\alpha}'$ is the microstructure incompatibility

Note: $T_\mu(x_\mu) = \bar{T}$ in 1st order homogenisation

- The Hill-Mandel condition with $\mathcal{P} = [\mathbf{P}, \boldsymbol{Q}^T]^T$

$$\bar{\mathcal{P}} \cdot \delta\bar{\mathcal{F}} = \frac{1}{\bar{V}} \int_{\bar{V}} \mathcal{P}_\mu \cdot \delta\mathcal{F}_\mu \; d\bar{V}$$

Translated to interfacial interpretation [Wu 2025]

- Fluctuations across $K = 0, 1, .., k$ interfaces with $i = 0,1..P$ phases

$$\mathcal{F}_i = \bar{\mathcal{F}} + \frac{1}{V_i} \sum_{\forall\, \Gamma_k^i \neq \emptyset} s_{i,k} \boldsymbol{N}_k \odot \boldsymbol{\alpha}'$$

where $s_{i,k}$ is the surface coefficient, $\boldsymbol{N}_k$ is the normal to the interface and $\boldsymbol{\alpha}'$ is the 4-dimensional DOF

- Weak form of the Hill-Mandel condition

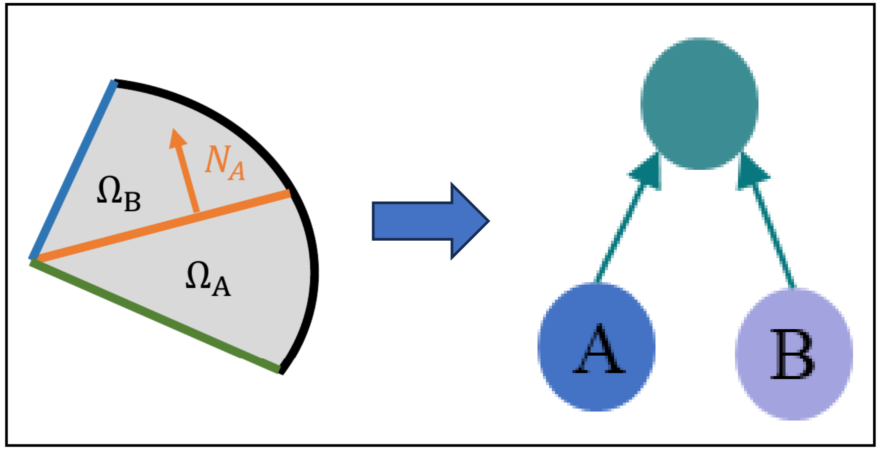
$$\left[\sum_k \left(\sum_i v_i \mathcal{P}_i s_{i,k}\right) \cdot \boldsymbol{N}_k\right] \cdot \; \delta\boldsymbol{\alpha}' = 0$$

DMN for a 2-scale problem with 2 phases

- For 2 solid phases **A** and **B** in local frames, $s_{\mathrm{A,B}} = -s_{\mathrm{B,A}}$ akin to laminate theory [Liu 2019], the strains:

$$\boldsymbol{\mathcal{F}}_A = \overline{\boldsymbol{\mathcal{F}}} + \frac{1}{\nu_A} \boldsymbol{N}_A \odot \widehat{\boldsymbol{\alpha}} \qquad \Bigg| \qquad \boldsymbol{\mathcal{F}}_B = \overline{\boldsymbol{\mathcal{F}}} - \frac{1}{\nu_B} \boldsymbol{N}_A \odot \widehat{\boldsymbol{\alpha}}$$

where $\widehat{\boldsymbol{\alpha}} = \frac{s_{\mathrm{A,B}}}{\overline{V}} \boldsymbol{\alpha}'$.



- Solution to incompatibility DOF from weak form of Hill-Mandel – solve with Newton-Raphson

$$\Delta\widehat{\boldsymbol{\alpha}} = (\mathbb{K}^{-1}\mathbb{F}) \cdot \Delta\overline{\boldsymbol{\mathcal{F}}} + (\mathbb{K}^{-1}\mathbb{T})\Delta\overline{T}$$

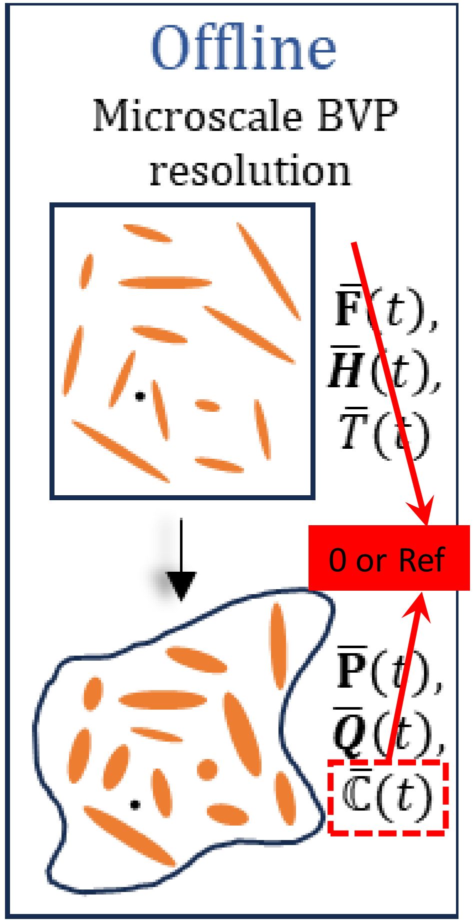
- Homogenised tangent operators

$$\partial\overline{\boldsymbol{\mathcal{P}}} = \boldsymbol{\mathcal{L}}(\mathbb{C}_{\boldsymbol{A}}, \mathbb{C}_{\boldsymbol{B}}, \mathbb{K}^{-1}\mathbb{F}) \cdot \partial\overline{\boldsymbol{\mathcal{F}}} + \boldsymbol{\mathcal{L}}_{\boldsymbol{T}}(\mathbb{C}_{\boldsymbol{A}}, \mathbb{C}_{\boldsymbol{B}}, \mathbb{K}^{-1}\mathbb{T})\, \partial\overline{T}$$

The matrices $\mathbb{K}$, $\mathbb{F}$ and $\mathbb{T}$ are functions $\mathbb{C}_{\boldsymbol{A}}, \mathbb{C}_{\boldsymbol{B}}$, ν_A and $\boldsymbol{N}_A$ (Note: $\nu_B = 1 - \nu_A$ and $\boldsymbol{N}_A$, the 3D normal, requires 2 angles)

∴ Trainable Topological Parameters are $\Lambda^3 = \{\nu_A, \boldsymbol{N}_A(\theta_A, \phi_A)\}$

DMN training protocol



Linear Elastic Training for a given RVE at <u>0 strains</u>

- Generate ‘n’ homogenised tangents (train + test) for random material parameters of 2 phases using **DNS** [Nguyen 2017]

$$\overline{\mathbb{C}}^{\mathrm{DNS}}_{s=0,\dots,N} = \mathrm{DNS}\left(\mathbb{C}^{i=0,1}_{s=0,\dots,N}\right)$$

- Material tensor evaluation at the apex node $(l = 0)$ for 2 phases

$$\overline{\mathbb{C}}^{\mathrm{DMN}}_{s=0,\dots,N} = \mathrm{DMN}\left(l = 0, \mathbb{C}^{i=0,1}_{s=0,\dots,N};\ \Lambda^{3}\right)$$

- Identify topological parameters from minimisation of loss function, knowing total phase volume fractions $(\nu_{i=0,1})$ – uses gradient descent from PyTorch

$$Loss\left(\overline{\mathbb{C}}^{\mathrm{DNS}}, \overline{\mathbb{C}}^{\mathrm{DMN}}\right) = \frac{1}{n}\sum_{\mathrm{n}} \frac{\left\|\overline{\mathbb{C}}^{\mathrm{DNS}} - \overline{\mathbb{C}}^{\mathrm{DMN}}_{s}(\dots;\Lambda^{3})\right\|}{\left\|\overline{\mathbb{C}}^{\mathrm{DNS}}\right\|}$$

Homogenised stacked tangent with relative scaling $(\lambda_1, \lambda_2, \lambda_3)$

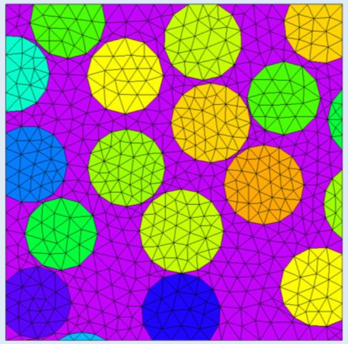
$$\overline{\mathbb{C}} \equiv \begin{bmatrix} \dfrac{\partial \overline{\boldsymbol{P}}}{\partial \overline{\boldsymbol{F}}} & \dfrac{\partial \overline{\boldsymbol{P}}}{\partial \overline{H}} & \lambda_1 \dfrac{\partial \overline{\boldsymbol{P}}}{\partial \overline{T}} \\ \dfrac{\partial \overline{\boldsymbol{Q}}}{\partial \overline{\boldsymbol{F}}} & \lambda_2 \dfrac{\partial \overline{\boldsymbol{Q}}}{\partial \overline{H}} & \lambda_3 \dfrac{\partial \overline{\boldsymbol{Q}}}{\partial \overline{T}} \end{bmatrix}$$

Note: All terms in matrix form.

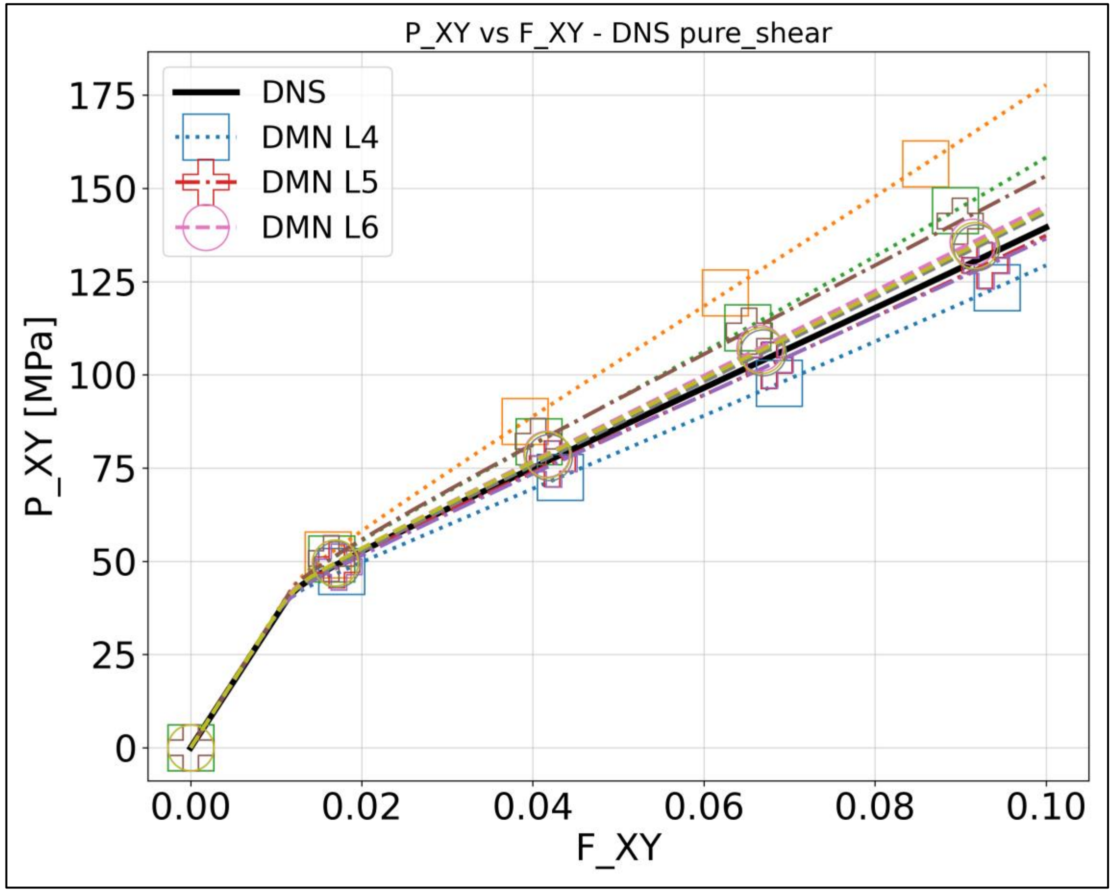
2 phase microscale DMN surrogate vs DNS 1

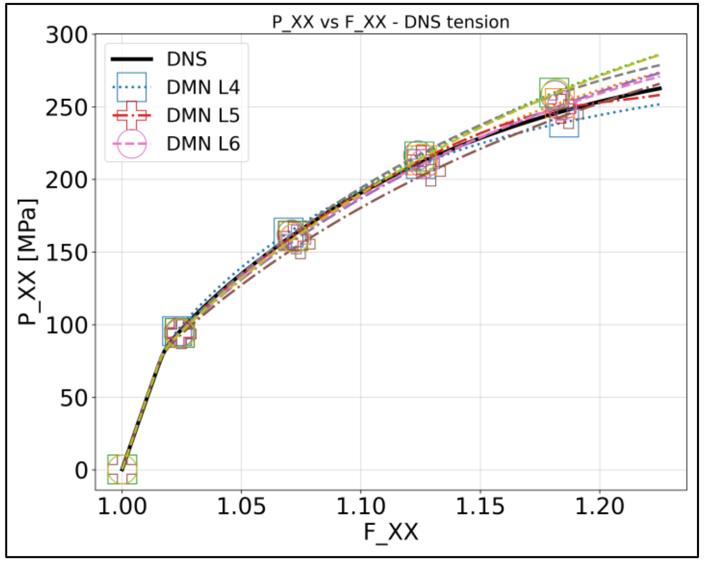
DNS on elastic fibre and J2 elasto-plastic resin UD composite RVE with PBC [Nguyen 2017] vs. Linear elastically trained **DMN** (same strain-path)

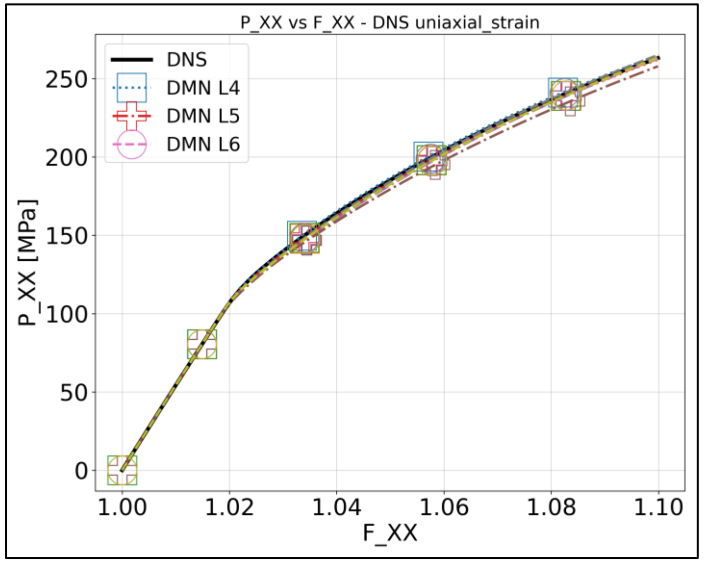
Offline Stage		
Data generation	30 mins/25 samples	
DMN Training	5 hours/1000 epochs L5	
Online	**FE**	**DMN**
Simulation	6 hours ~ 10% strain	5 mins L5



Note: Time per CPU



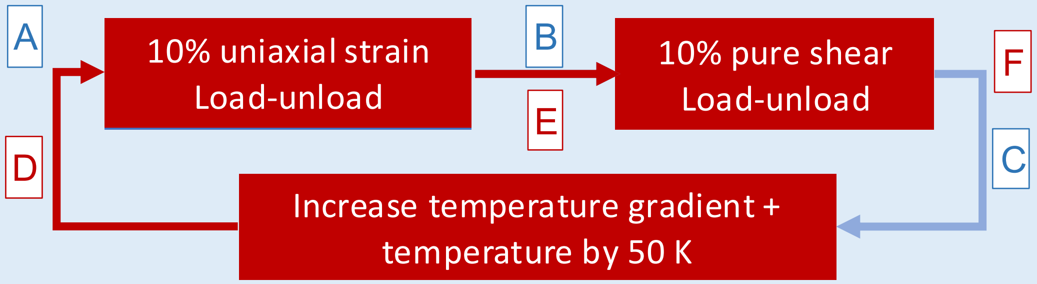




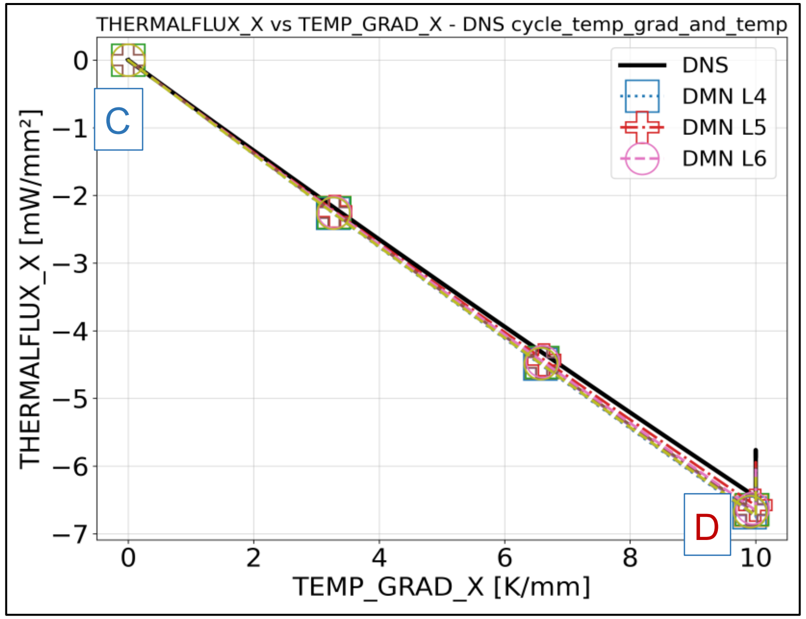
Vinyl ester and carbon fibre data from [Gupta 2020] and [Wong 2022], respectively

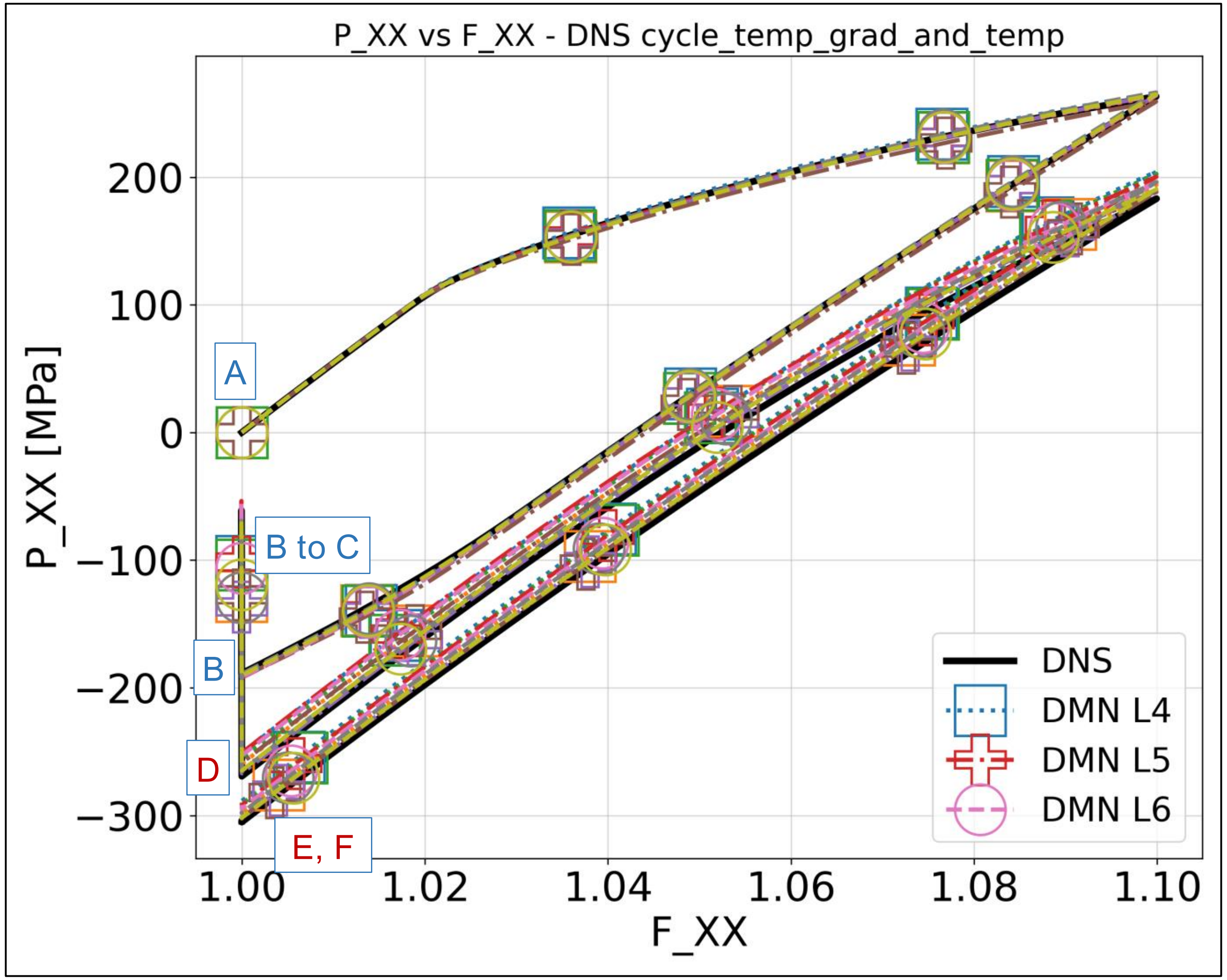
2 phase microscale DMN surrogate vs. DNS 2

Response in thermomechanical cyclic loading



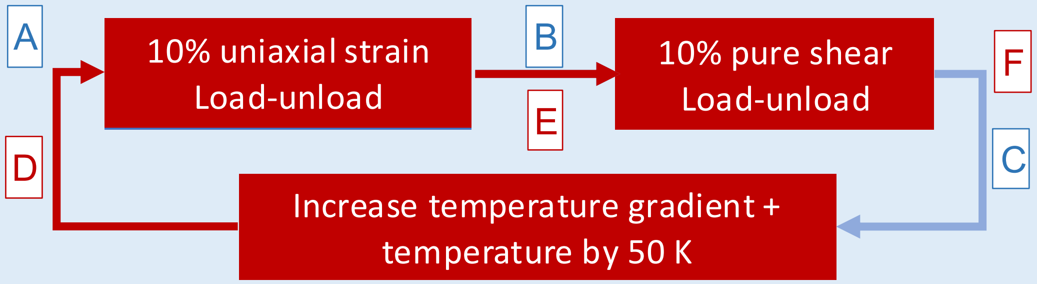
Online	FE	DMN
Simulation	~1 day	20 mins L5



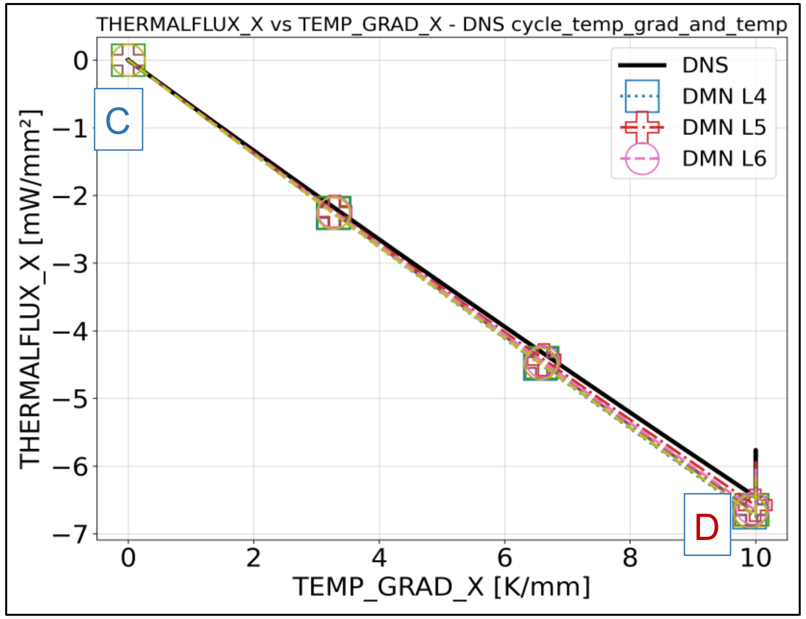


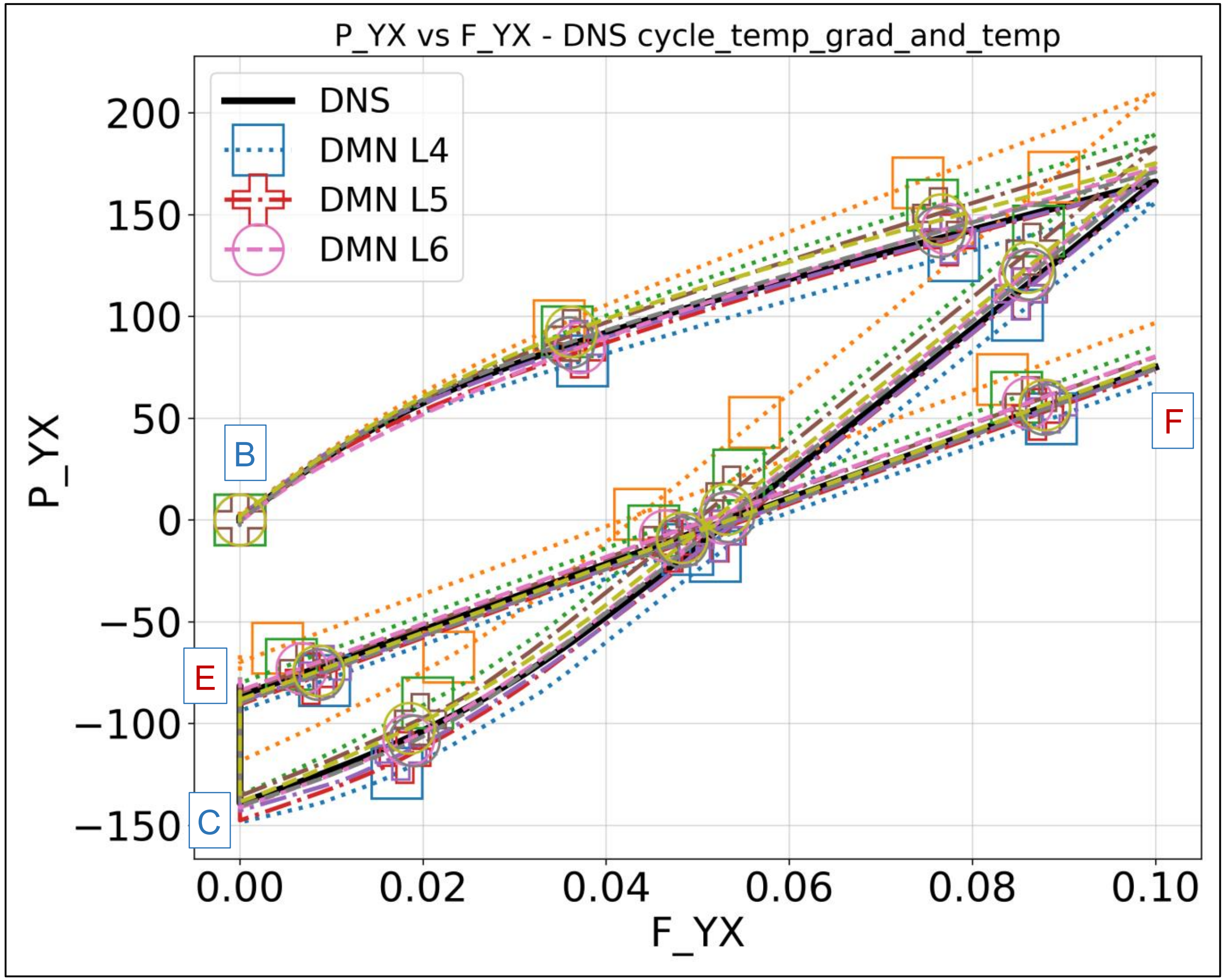
2 phase microscale DMN surrogate vs. DNS 2

Response in thermomechanical cyclic loading

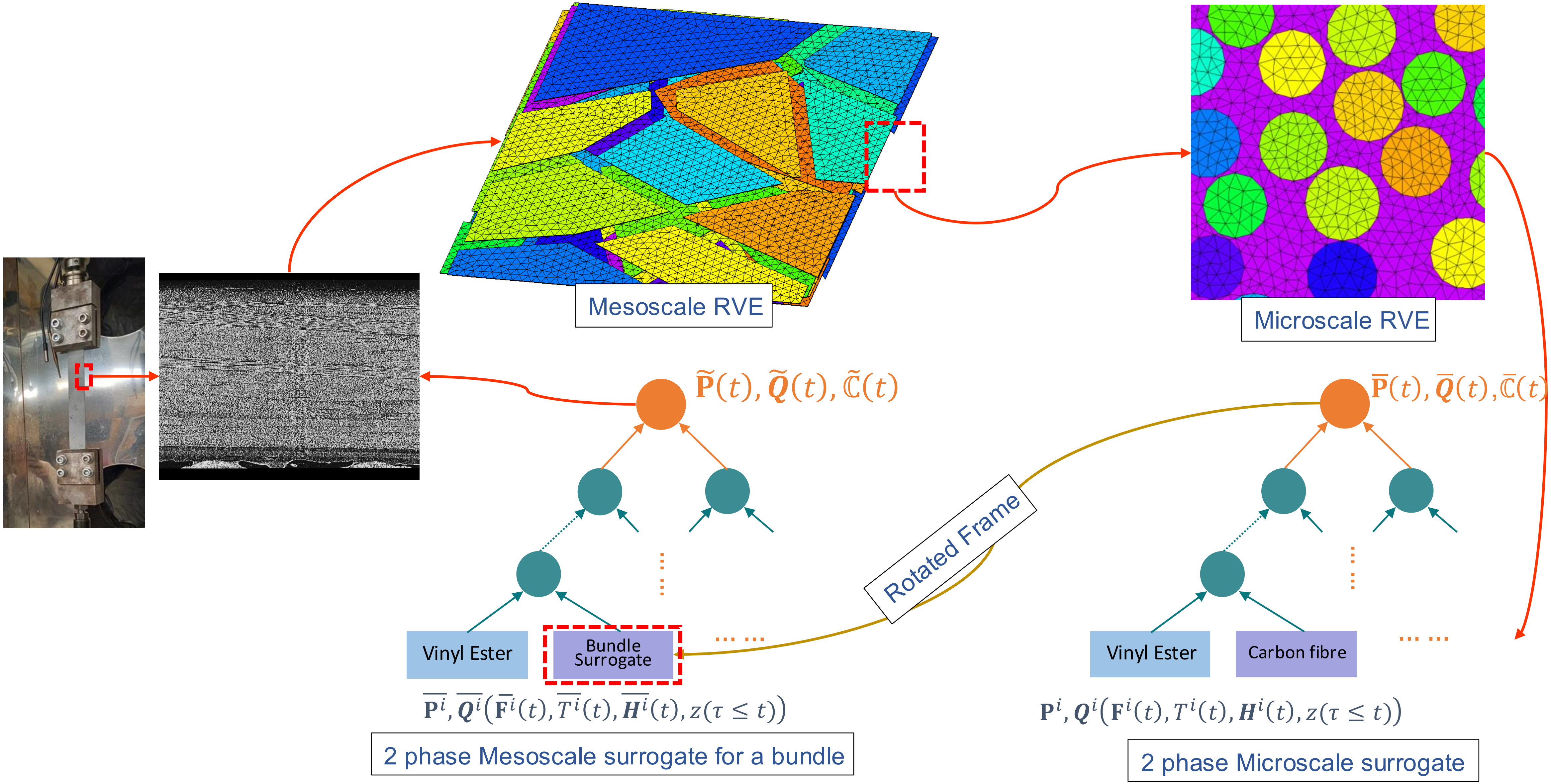


Online	FE	DMN
Simulation	~1 day	20 mins L5

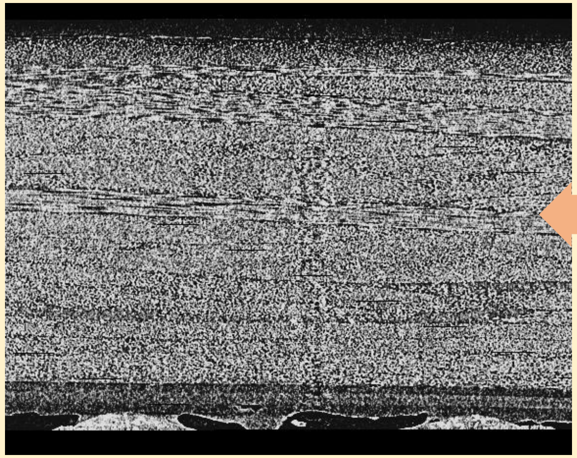




3 scale SMC problem with DMN surrogates

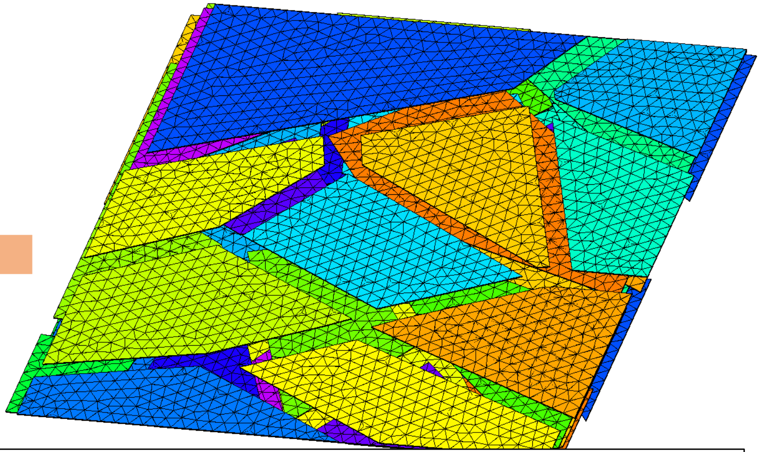


2-phase DMN with a locally oriented phase (under development)

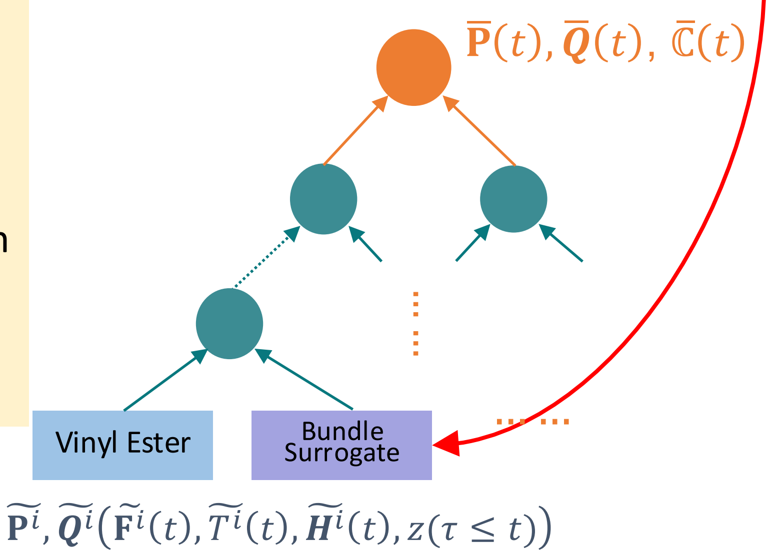


$$\mathbf{A} = \begin{bmatrix} 0.55 & 0 & 0 \\ 0 & 0.45 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Orientation vectors sampled from reconstructed ODF [Zulueta 2024] from 2nd order orientation tensor [Mohamedou 2019]



Each bundle has an orientation vector $\vec{e}_r$



Modified Training Protocol

- Random train + test data with RVE orientations on micro-DMN using **DNS**

$$\tilde{\mathbb{C}}^{\mathrm{DNS}}_{s=0,\ldots,N} = \mathrm{DNS}\left(\mathbb{C}^0_s, \mathcal{R}\left(\overline{\mathbb{C}}^{1\approx\mathrm{DMN}}_s\right)\right)$$

where $\mathcal{R} = \mathcal{R}(\vec{e}_r)$ is a rotation operator

- DMN stiffness evaluation by capturing orientation as a microstructural feature

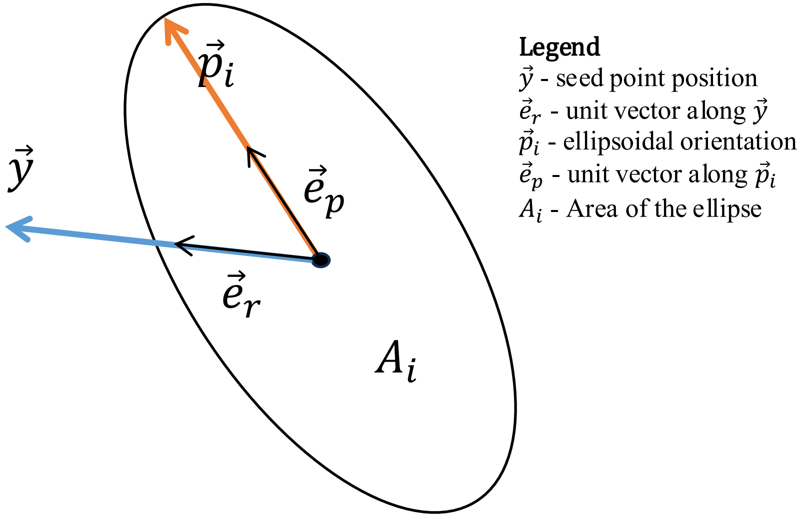
$$\tilde{\mathbb{C}}^{\mathrm{DMN}}_{s=0,\ldots,N} = \mathrm{DMN}\left(\mathbb{C}^0_s, \overline{\mathbb{C}}^{1\approx\mathrm{DMN}}_s;\ \Lambda^6\right)$$

- Extended topological parameters Λ^6 with 3 Euler angles for each Bundle surrogate node

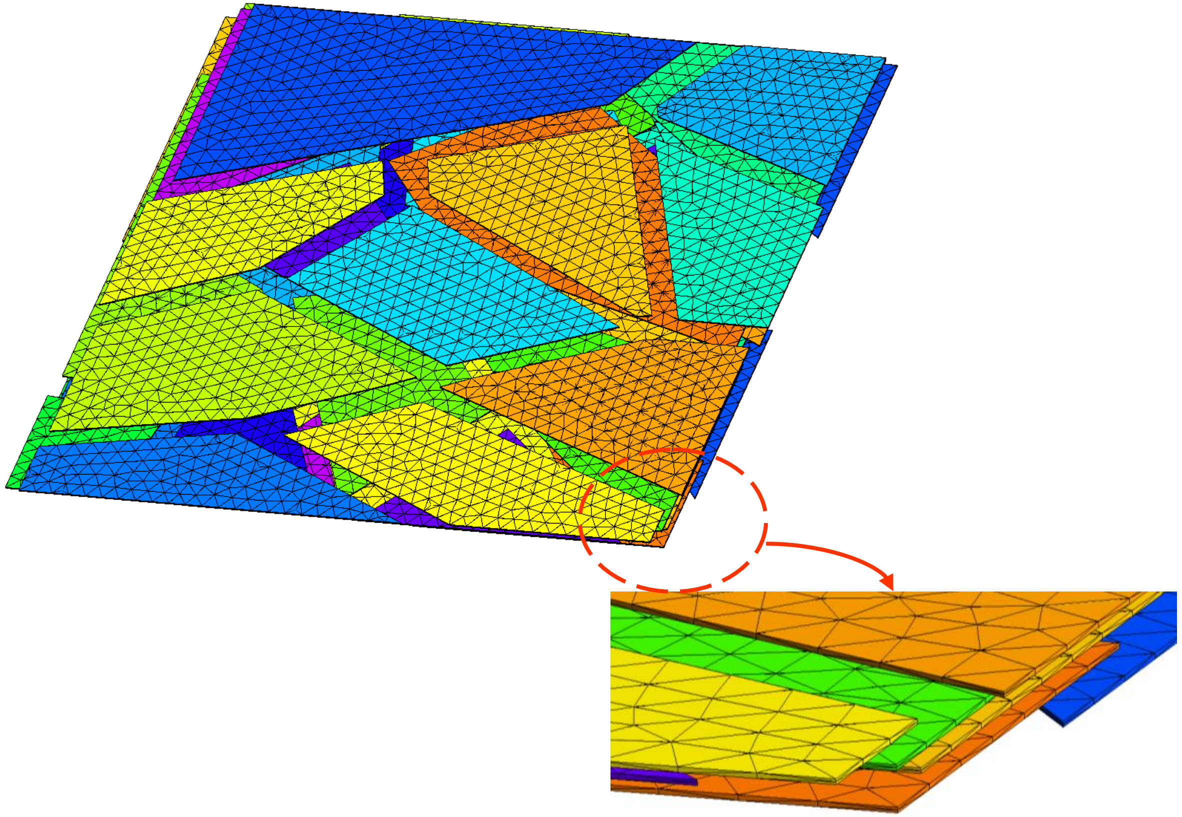
$$\therefore \Lambda^6 = \{\nu_A, \boldsymbol{N}_A(\theta_A, \phi_A), \mathfrak{R}(\alpha, \beta, \gamma)\}$$

where $\mathfrak{R}$ is a reduced set of $\mathcal{R}$

Mesoscale RVE using anisotropic Voronoi algorithm



2D ellipsoidal field [Nuland 2021]



Ellipsoidal velocity field in 2D

$$v_i(\vec{y}) = \sqrt{\frac{A_i}{\pi\|\vec{p}_i\|}}\left[1 + \left(\frac{1}{\|\vec{p}_i\|^2} - 1\right)\left(\vec{e}_p \cdot \vec{e}_r\right)^2\right]^{-\frac{1}{2}}$$

- Boundaries based on growth times – radial distance
- Anisotropy from orientation and aspect ratio – Applied to SMC bundles

Anisotropic Voronoi Cells

- Random seeds using Poisson disk sampling
- Convex polygonisation using convex-hull algorithm
- Shrunk and stacked to create layered structure (resin fills the gaps – not shown)

Conclusions and Perspectives

- Generalized Deep Material Network methodology for thermomechanical coupling – Shown to work!
- Extension to DMNs with local phase orientations – New training protocol!
- Incorporation of viscous and dissipative effects
- Incorporation of non-local damage at the micro level with thermal effects

References

[MDC Mould 2020] www.zjmdc.com/IndustryNews/SMC-sheet-molding-compound-production-process.html

[Ebrahimian 2024] Ebrahimian, F., et al. "Optimization of precharge placement in sheet molding compound process." *International Journal of Material Forming* 17.4 (2024): 34

[Zulueta 2024] Zulueta K., et al. "Effects of temperature on the anisotropic mechanical properties and failure mechanisms of Sheet Molding Compounds." Composites Part A: Applied Science and Manufacturing 186 (2024): 108424.

[Fidler 2024] Fidler A. G., et al. "Carbon Fibre Reinforced Sheet Moulding Compound in Brakes: Manufacturing and Testing of a Lightweight Motorcycle Brake Calliper." *EuroBrake 2024: Europe's Braking Technology Conference & Exhibition*. Fédération Internationale des Sociétés d'Ingénieurs des Techniques de l'Automobile FISITA, 2024

[Liu 2019] Liu Z., et al. "A deep material network for multiscale topology learning and accelerated nonlinear modeling of heterogeneous materials." *Computer Methods in Applied Mechanics and Engineering* 345 (2019): 1138-1168

[Nguyen 2022] Nguyen V.-D., L. Noels. "Micromechanics-based material networks revisited from the interaction viewpoint; robust and efficient implementation for multi-phase composites." European Journal of Mechanics-A/Solids 91 (2022): 104384

[Wu 2025] Wu L., L. Noels. "Stochastic deep material networks as efficient surrogates for stochastic homogenisation of non-linear heterogeneous materials." *Computer Methods in Applied Mechanics and Engineering* 441 (2025): 117994

[Nguyen 2017] Nguyen V.-D., L. Wu, and L. Noels. "Unified treatment of microscopic boundary conditions and efficient algorithms for estimating tangent operators of the homogenized behavior in the computational homogenization method." Computational Mechanics 59 (2017): 483-505

[Gupta 2020] Gupta, J., et al. "A comparative study between epoxy and vinyl ester CF-SMC for high volume automotive composite crash structures." *Composite Structures* 244 (2020): 112299

[Wong 2022] Wong, S., et al. "Direct Measurement of the Transverse Modulus of Carbon Fibres." *Experimental Mechanics* 62.5 (2022): 769-778

[Mohamedou 2019] Mohamedou, M, et al. "Bayesian identification of mean-field homogenization model parameters and uncertain matrix behavior in non-aligned short fiber composites." *Composite Structures* 220 (2019): 64-80

[Nuland 2021] Van Nuland, T. F. W., et al. "A novel 3D anisotropic Voronoi microstructure generator with an advanced spatial discretization scheme." *Modelling and Simulation in Materials Science and Engineering* 29.8 (2021): 085014

LIÈGE université
Sciences Appliquées

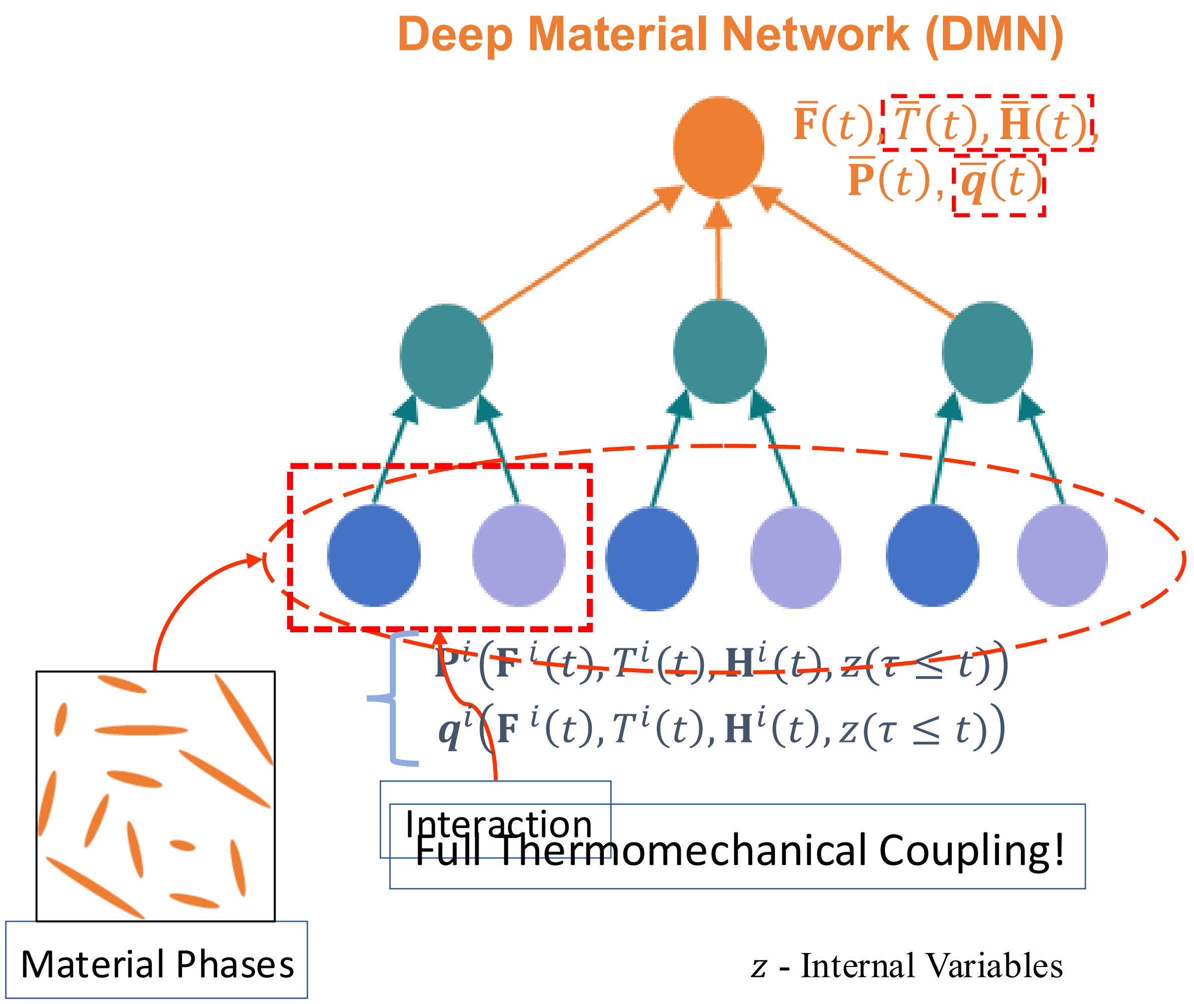
Thank you for your attention!

5th International Conference on Computational Methods for Multi-scale, Multi-uncertainty and Multi-physics Problems
CM3P 2025
July 1-4, 2025, Porto, Portugal

U.-K. Jinaga*
ujwalkishore.jinaga@uliege.be
Computational & Multiscale Mechanics of Materials (CM3),
B52, Allée de la découverte 9, B4000 Liège, Belgium
http://www.ltas-cm3.ulg.ac.be/

This research has been funded by the Walloon Region under the agreement no. 2010092-CARBOBRAKE in the context of the M-ERA.Net Join Call 2020. Funded by the European Union under the Grant Agreement no. 101102316. Views and opinions expressed are those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the granting authority can be held responsible for them.

Appendix - Deep Material Network (DMN)

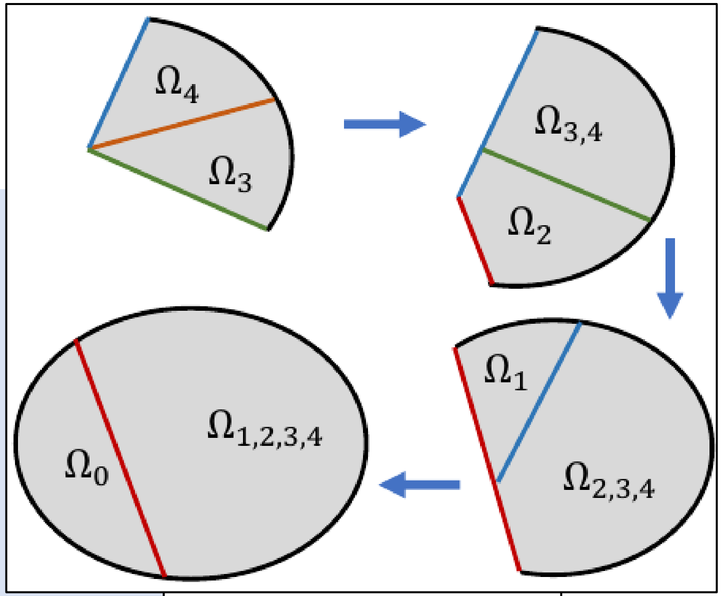


State of the art

- [Liu 2019] Isothermal finite-strain
- [Gajek 2021-22] Thermomechanical small-strain, isothermal application to real structure
- [Nguyen 2021-22] Interaction based, Isothermal finite-strain (developed in CM3)
- [Wu 2025] Stoichiometric, Interface interpretation, Isothermal small-strain (developed in CM3)

Lack of finite-strain thermomechanical DMN surrogate modelling!

Appendix - Interface-based Interpretation of DMN



Network of 2-phase interfaces [Wu 2025]

- Link homogenised combined gradient to nodes
  - $\boldsymbol{\mathcal{F}} = [\boldsymbol{F}, H^T]^T$ in the mapping

$$\bar{\boldsymbol{\mathcal{F}}} + \sum_{k=0}^{M-1} \alpha^{i,k}\, \boldsymbol{a}^k \otimes \boldsymbol{N}^k = \boldsymbol{\mathcal{F}}^i, \quad i = 0 \dots 9$$

  - $\bar{T} = T^i$ limitation of 1st order homogenisation
- Weak form of Thermomechanical Hill-Mandel Condition
  - $\boldsymbol{\mathcal{P}} = [\boldsymbol{P}\ \boldsymbol{q}^T]^T$

$$\bar{\boldsymbol{\mathcal{P}}} : \delta\bar{\boldsymbol{\mathcal{F}}} = \sum_i W^i \boldsymbol{\mathcal{P}}^i : \delta\boldsymbol{\mathcal{F}}^i \;\Rightarrow\; \left[\sum_k \left(\sum_i W^i \boldsymbol{\mathcal{P}}^i \alpha^{i,k}\right) \cdot \boldsymbol{N}^k\right] \cdot \delta\boldsymbol{a}^k = 0$$

$\Rightarrow$ *Constitutive behaviours:* $\boldsymbol{\mathcal{P}}^p(t) = \boldsymbol{\mathcal{P}}^p\left(\boldsymbol{\mathcal{F}}^i(t), T(t);\ \boldsymbol{Z}(\tau \le t)\right)$

if node i ∈ phase p for material p=0 or p=1

- Homogenized dependant set from volumetric averaging

$$\bar{\boldsymbol{\mathcal{P}}} = \sum_i W^i \boldsymbol{\mathcal{P}}^i$$

Appendix - DMN Training

Thermomechanical homogenisation of composite systems

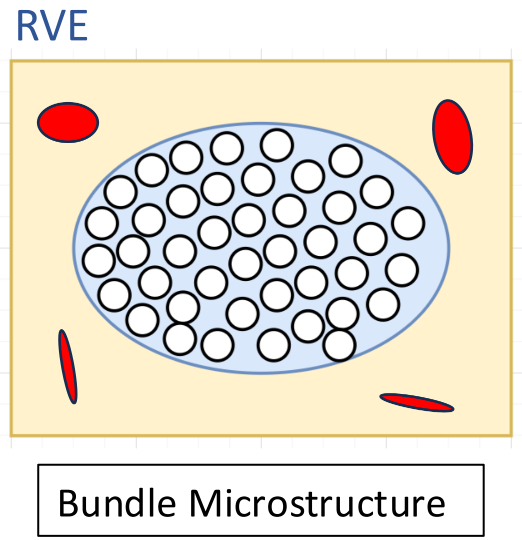
- **Offline training**

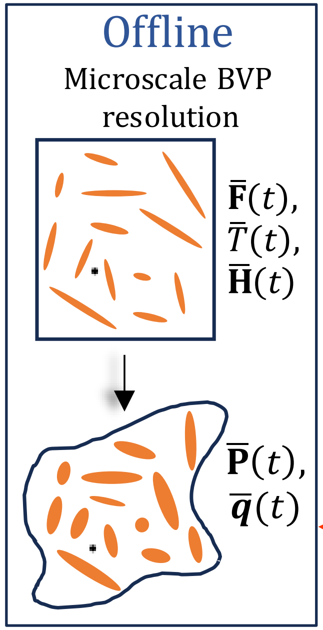
  -> TVE - Random generation of $\mathbb{C}$

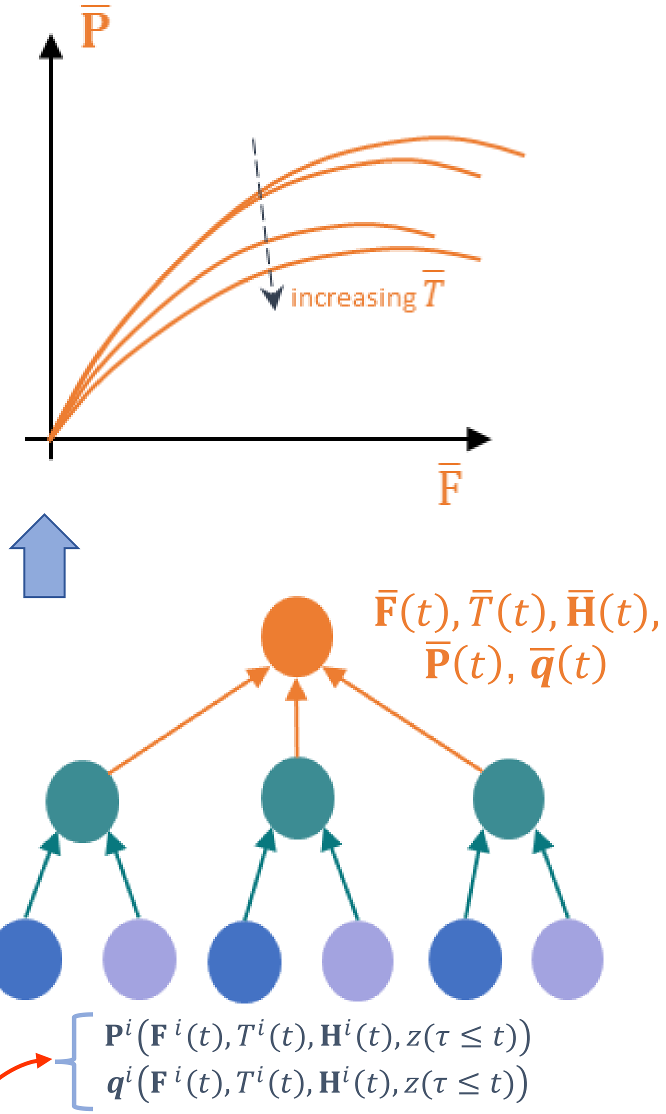
  -> TVP - Random generation of stress vs. strain loading paths

  Fitting parameters as Microstructural descriptors

- Training to minimise a loss function using gradient descent (PyTorch)

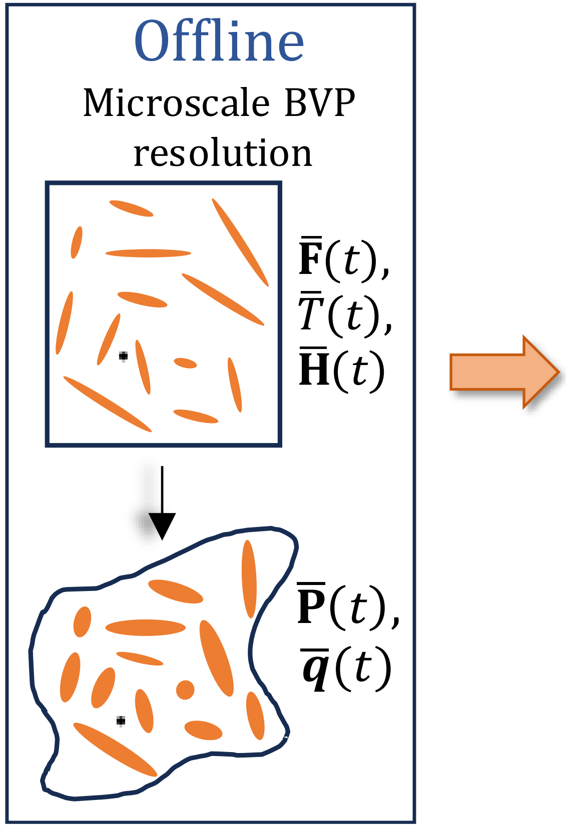






Constitutive Material Laws

Appendix - Thermomechanical Tangents in DMN



Offline Data

- Constitutive behaviour for the combined “stress” at initialisation:

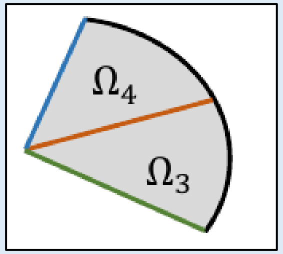
$$\Delta\mathcal{P} = \Delta\mathcal{P}(\Delta\mathcal{F}, \Delta T)$$

- Homogenised stacked tangent (with relative scaling) for training:

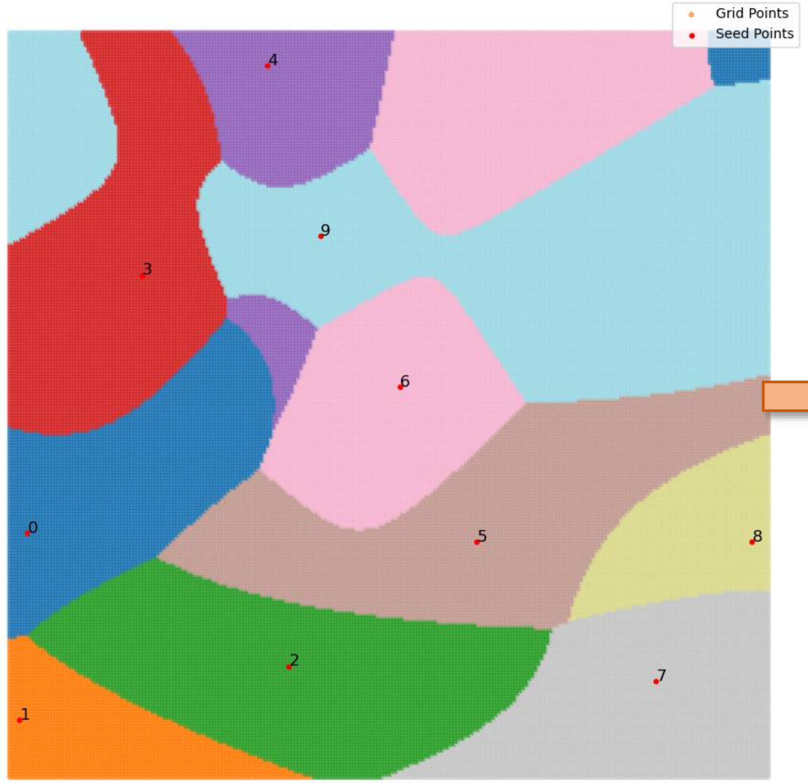
$$\left[\frac{\partial\bar{\mathcal{P}}}{\partial\bar{\mathcal{F}}}, \frac{\partial\bar{\mathcal{P}}}{\partial T}\right] \equiv \begin{bmatrix} \frac{\partial\bar{\boldsymbol{P}}}{\partial\bar{\boldsymbol{F}}} & \frac{\partial\bar{\boldsymbol{P}}}{\partial\bar{H}} & \frac{\partial\bar{\boldsymbol{P}}}{\partial\bar{T}} \\ \frac{\partial\bar{q}}{\partial\bar{\boldsymbol{F}}} & \frac{\partial\bar{q}}{\partial\bar{H}} & \frac{\partial\bar{q}}{\partial\bar{T}} \end{bmatrix}$$

- To train the DMN parameters:

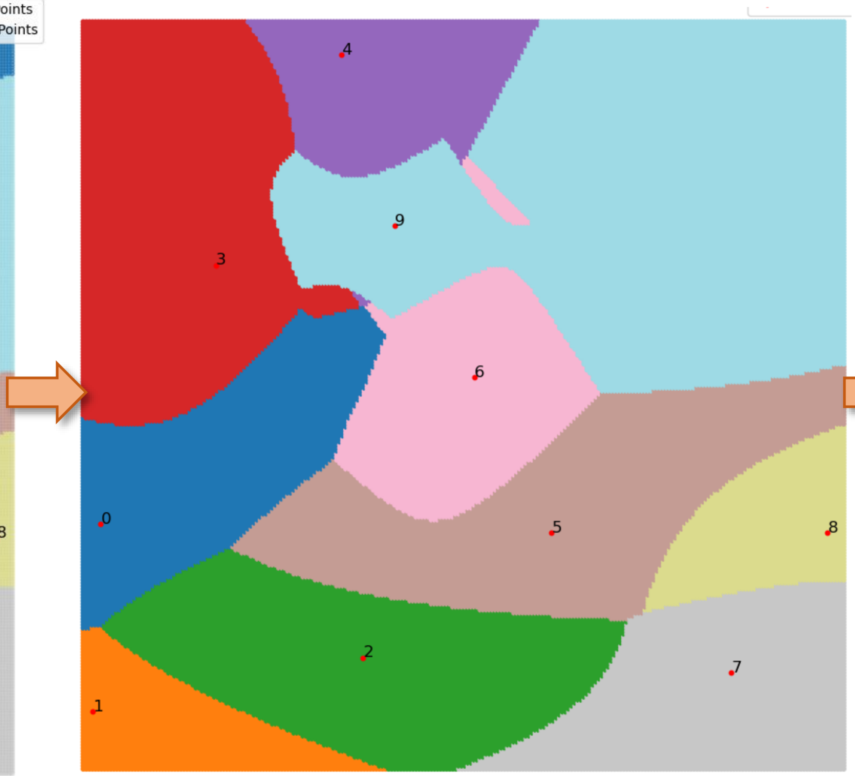
$\alpha^{i,k}$ - interface coefficients
$\boldsymbol{N}^k$ - interface normal
W^i - weights ~ volume fractions



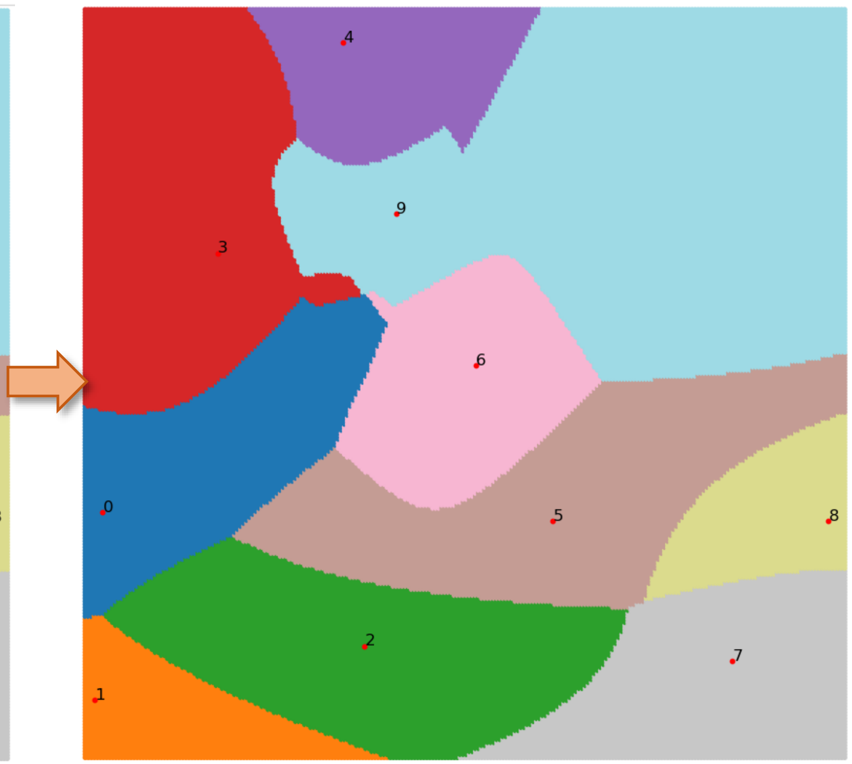
Appendix - Anisotropic Voronoi algorithm 1
- Robust Methodology for Domain Refinement



Initial assignment using Ellipsoidal growth field causes islandification.

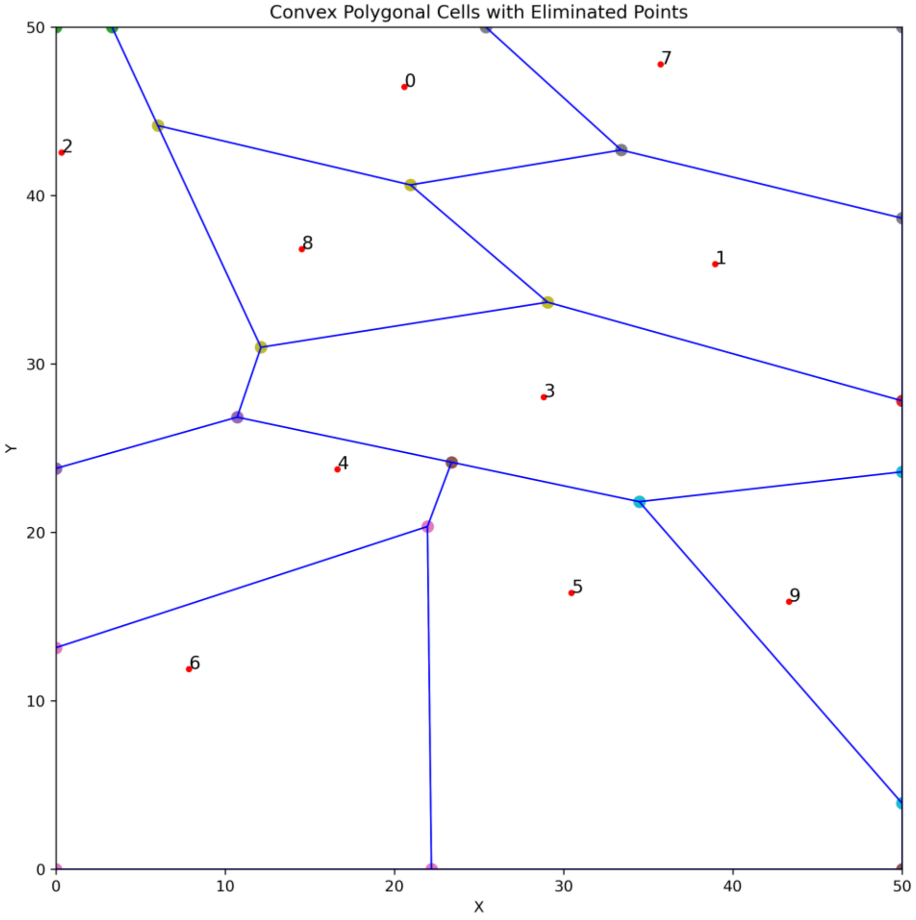


Reassignment 1 - Identify islands by KD Tree split-planes and reassign using distance from domain centre of mass.

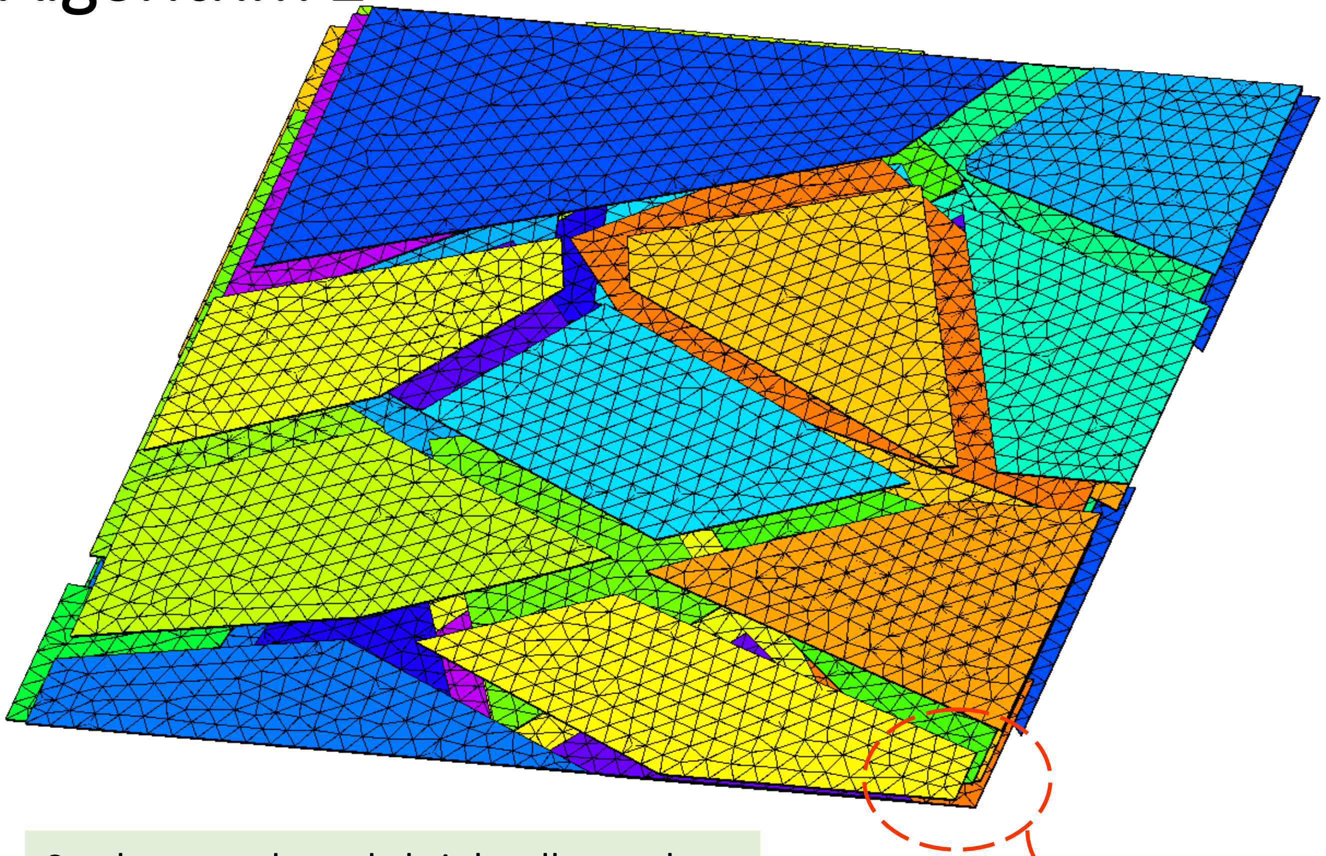


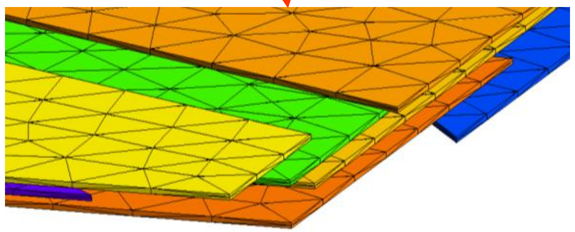
Reassignment 2 - Re-identify islands by KD and re-reassign to domain of the closest seed to parent.

Appendix - Anisotropic Voronoi Algorithm 2
- Polygonisation and layered stacking



Polygonisation - Find domain junctions and form polygons using Convex Hull algorithm.





Stack - extrude and shrink cells, stack layers, Boolean to form a negative space for polymer (not shown).